The Theory of Intermolecular Forces

by Anthony J. Stone (Oxford University Press, 1996)
reprinted in paperback, with corrections, 1997
and with further corrections, 2000

Unfortunately there were a number of errors in the original hardback edition. Some of these were corrected in the 1997 paperback reprint, and a further batch were corrected in the 2000 reprint. A few further corrections have since come to light. All these corrections are listed here.

I would be grateful to be told of any further errors that you may find. I will endeavour to keep this list up to date; please check http://www-stone.ch.cam.ac.uk/timf/corrections.pdf before reporting further errors. The last corrections were added on 29 August 2008.

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The following corrections need to be made to the 1996 hardback edition, but were included in later editions:

p. 81, eq. (6.1.3):
This equation (starting on p. 80) should read as follows:

$$\begin{aligned} U_{\text{er}} &= \frac{S^2}{1-S^2}\left\langle a(1)b(2)\middle|-\frac{1}{r_{A2}}-\frac{1}{r_{B1}}+\frac{1}{r_{12}}\middle|a(1)b(2)\right\rangle \\ &\quad -\frac{1}{1-S^2}\left\langle a(1)b(2)\middle|-\frac{1}{r_{A2}}-\frac{1}{r_{B1}}+\frac{1}{r_{12}}\middle|a(2)b(1)\right\rangle \\ &= -\frac{S^2}{1-S^2}\left[\left\langle b\middle|\frac{1}{r_A}|b\right\rangle+\left\langle a\middle|\frac{1}{r_B}|a\right\rangle-\left\langle a(1)b(2)\middle|\frac{1}{r_{12}}\middle|a(1)b(2)\right\rangle\right] \\ &\quad +\frac{1}{(1-S^2)}\left[S\left\langle a\middle|\frac{1}{r_A}+\frac{1}{r_B}\middle|b\right\rangle-K_{ab}\right]. \end{aligned} \tag{6.1.3}$$

p. 91, l. 11:
The citation of Jeziorski & Kołos (1977) is incorrect here (though they are correctly cited on l. 13); this one should be Jeziorski *et al.* (1978).

p. 231, Table E.5:
The right-hand-side of every entry should be divided by 3.

p. 234, Table F.1:
The following entries should be corrected as shown:

41c	00	$R^{-5}.\frac{1}{4}\sqrt{10}(7r_x^a r_z^{a3}-3r_x^a r_z^a)$
41s	00	$R^{-5}.\frac{1}{4}\sqrt{10}(7r_y^a r_z^{a3}-3r_y^a r_z^a)$

The following corrections were included in the 2000 paperback reprint, but need to be made to earlier editions:

p. 15, top line:
The statement that the other components 'are all zero' is nonsense. (I must have been thinking about the spherical components when I wrote that.) For the molecules previously discussed, which are all linear or symmetric tops, $\Theta_{xx}=\Theta_{yy}=-\frac{1}{2}\Theta_{zz}$, and all of these will be nonzero.

p. 24, 6 lines below (2.3.14):
The anisotropy $\Delta\alpha$ should be $\alpha_{zz}-\frac{1}{2}(\alpha_{xx}+\alpha_{yy})$.

pp. 25–26:
In eqs. (2.4.2) and (2.4.3) and the two preceding equations, the denominator in the second term should be $(W_n-W_0)^2$. not W_n-W_0.

p. 27:
In eq. (2.5.6), there is a missing closing parenthesis at the end of the numerator of the last two lines. The ω_{k0} in the numerator of the last line should be ω. In eq. (2.5.7) there is a missing closing bracket at the end of the numerator.

p. 38, eqs. (3.1.9) and (3.1.10):
There is an error of sign in the last line of each of these equations, which should read:

$$\begin{aligned} F^A_\alpha(\mathbf{B}) &= -\nabla_\alpha V^A(B) \\ &= -T_\alpha q + T_{\alpha\beta}\hat{\mu}_\beta - \frac{1}{3}T_{\alpha\beta\gamma}\hat{\Theta}_{\beta\gamma} + \cdots \\ &\quad \cdots - \frac{(-1)^n}{(2n-1)!!}T^{(n+1)}_{\alpha\beta\ldots\nu\sigma}\hat{\xi}^{(n)}_{\beta\gamma\ldots\nu\sigma} - \cdots, \end{aligned} \tag{3.1.9}$$

and for the field gradient,

$$\begin{aligned} F^A_{\alpha\beta}(\mathbf{B}) &= -\nabla_\alpha\nabla_\beta V^A(B) \\ &= -T_{\alpha\beta} q + T_{\alpha\beta\gamma}\hat{\mu}_\gamma - \frac{1}{3}T_{\alpha\beta\gamma\delta}\hat{\Theta}_{\gamma\delta} + \cdots \\ &\quad \cdots - \frac{(-1)^n}{(2n-1)!!}T^{(n+2)}_{\alpha\beta\ldots\nu\sigma\tau}\hat{\xi}^{(n)}_{\gamma\delta\ldots\nu\sigma\tau} - \cdots. \end{aligned} \tag{3.1.10}$$

I believe that the subsequent equations are correct as to sign.

p. 53:
The l.h.s. of eq. (4.2.1) should refer to U^B_{ind}, not U^A_{ind}. In the line below the equation, replace ‘merely’ by ‘minus’.

p. 77:
in l. 7 of the paragraph numbered 2, the integral should include a factor r_{12}^{-1}.

p. 183:
There should be no sum over B in eq. (11.7.10).

p. 188:
Eq. (12.1.4) is better expressed in the form

$$f_n = \frac{2}{3}\frac{\hbar\omega_n}{E_h}\frac{\left|\langle 0|\hat{\mu}|n\rangle\right|^2}{e^2 a_0^2} \tag{12.1.4}$$

where E_h is the Hartree energy. This form is independent of unit system and is manifestly dimensionless. In the same way, eq. (12.1.5) is better written as

$$S_k = \sum_n f_n \left(\frac{\hbar\omega_n}{E_h}\right)^k \tag{12.1.5}$$

while the expression for S_{-2} three lines lower is better written as $S_2 = \overline{\alpha}/4\pi\varepsilon_0 a_0^3$.

p. 199:
There is a superfluous minus sign in eq. (12.3.10), which should read

$$\mathrm{i}\frac{\partial\Psi}{\partial t} = -\sum_k \nabla_k^2\Psi + V\Psi \tag{12.3.10}$$

p. 213:
There is an error in the first expression given for R_{20}, which should be $R_{20}(\mathbf{r}) = \frac{1}{2}(3z^2 - r^2)$.

p. 225:
The conversion factor table for dipole moment units has a typographical error: in the second row of numbers, 1 Debye should be shown as equal to $3.33564095 \times 10^{-30}\,\mathrm{C\,m}$, and (of course) to 1 Debye.

p. 233, Table F.1:
The following entries should be corrected as shown:

$31c$	00	$R^{-4}.\frac{1}{4}\sqrt{6}r_x^a(5r_z^{a2}-1)$
$31s$	00	$R^{-4}.\frac{1}{4}\sqrt{6}r_y^a(5r_z^{a2}-1)$
$33c$	1β	$R^{-5}.\frac{1}{4}\sqrt{10}(7r_x^{a3}r_\beta^b+3(r_x^{a2}-r_y^{a2})c_{x\beta}-21r_x^ar_y^{a2}r_\beta^b-6r_x^ar_y^ac_{y\beta})$

The following corrections need to be made to all versions up to and including the 2000 reprint:

p. 24, first paragraph of **S**2.3.1:
The symbol Å for Ångstrom is twice misprinted as **r**A.

p. 32:
The last line of **S**2.6 should read
... the symbol C denotes $\frac{1}{5}C_{\alpha\beta,\alpha\beta}=\frac{1}{10}\sum_\kappa\alpha_{2\kappa,2\kappa}$.

p. 54, below eqn (4.2.2):

In the third line below the equation, there is a missing factor of $-\frac{1}{2}$. It should read:
... and the induction energy is $-\frac{1}{2}q^2\alpha_{zz}^B/((4\pi\varepsilon_0)^2z^4)$.

p. 62, eq. (4.3.22):
The factor $\hbar/\pi$ should be $\hbar/2\pi$.

p. 140, eqs. (8.7.1) and (8.7.2):
The factor $\hbar/\pi$ should be $\hbar/2\pi$.

p. 188, eq. (12.1.6): This equation should read

$$\overline{\alpha}(iv)=4\pi\varepsilon_0a_0^3\frac{E_h^2}{\hbar^2}\sum_{k=1}^N\frac{\tilde{f}_k}{\tilde{\omega}_k^2+v^2},$$

p. 214, eq. (B.1.7): These equations apply for $m>0$.

p. 229, Table E.2:
The following entries should be corrected as shown:

Ω_{xyy}	$-\sqrt{\frac{5}{8}}Q_{33c}-\sqrt{\frac{1}{24}}Q_{31c}$
Ω_{yyy}	$-\sqrt{\frac{5}{8}}Q_{33s}-\sqrt{\frac{3}{8}}Q_{31s}$
Φ_{xxxx}	$\frac{3}{8}Q_{40}-\frac{1}{4}\sqrt{5}Q_{42c}+\frac{1}{8}\sqrt{35}Q_{44c}$
Φ_{xxyy}	$\frac{1}{8}Q_{40}-\frac{1}{8}\sqrt{35}Q_{44c}$
Φ_{yyyy}	$\frac{3}{8}Q_{40}+\frac{1}{4}\sqrt{5}Q_{42c}+\frac{1}{8}\sqrt{35}Q_{44c}$
Φ_{xxxz}	$\frac{1}{16}(-3\sqrt{10}Q_{41c}+\sqrt{70}Q_{43c})$